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Multi-scale Computer Aided Synthesis–Design–Intensification Method for Sustainable Hybrid Solutions

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Process synthesis-design refers to identification of the processing route to reach a desired product from a specified set of raw materials, design of the operations involved in the processing route along with calculations of utility requirements, waste generations and emissions to the environment, while process intensification refers to strategy by which new processes can be designed or existing processes can be redesigned to be more efficient, compact and sustainable. Therefore, in order to achieve sustainable process design it would be logical to perform process synthesis-design and process intensification together.

In this work, a four stage hierarchical decomposition solution strategy is proposed to generate sustainable hybrid solutions. The framework operates at different scales, the unit operations scale, task scale and phenomena scale. In stage1, process synthesis is performed (at the unit operations scale) using computer -aided flowsheet design method (CAFD) (Tula et al, 2015), which applies principles of computer-aided molecular design to the synthesis and design of process flowsheets. That is, use process-groups representing different unit operations (reactor, distillation, flash, crystallization, etc.), bonds representing streams and/or recycles, rules for chemical feasibility also representing process flowsheet feasibility and sum of group contributions representing the performance of the flowsheet which can later be used to quickly screen the alternatives and to generate the optimal processing route. In stage 2, the base case design is first established based on the generated processing route. This base case design is further analyzed to identify process hotspots (process bottlenecks) using a comprehensive analysis, consisting indicator based methods for economic, sustainability (Carvalho et al., 2013) and life cycle assessments (Kalakul et al., 2014). These indicators corresponding to the hotspots are translated to design targets that are targeted in the next stage to achieve more sustainable design. In stage 3, integrated task phenomena based synthesis intensification method is applied (Babi et al., 2015). The main idea here is to generate all the phenomena involved in the process by breaking the tasks involved into corresponding phenomena. Later these phenomena scale units are combined using combination rules in order to generate new and/or existing unit operations that constitute the (more sustainable) flowsheet alternatives which satisfy the intensification design targets. In this way, truly predictive and innovative hybrid solutions are generated much in the same way as atoms are combined to form molecules with desired properties (that is, analogous to computer-aided molecular design) which are otherwise could not be found from the higher scales. In the final stage, detailed model based simulations and/or experiments are performed to verify and compare the new solutions.

In this presentation, the multi-scale computer-aided framework will be presented together with the corresponding databases, computer- aided methods and tools needed to achieve sustainable synthesis-design-intensification. The framework will be highlighted through different case studies generating hybrid solutions for simple separation synthesis to complete flowsheet synthesis.

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